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Towards Closing the Autonomous Loop at Multiple Facilities: Developing Web-based User Interfaces and Data Infrastructure for Autonomous Experiments and Machine Learning Workflows

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Autonomous experiments rely on the seamless integration of control systems, data acquisition, data processing, and optimization frameworks. However, the inherent variability in facility- or beamline-specific infrastructure components poses a challenge for developing more generalizable setups and presents an obstacle for replication studies and cross-facility experiments.
This project focuses on establishing a robust infrastructure for autonomous small- and wide-angle scattering experiments at two different synchrotrons: x-ray scattering beamlines at the Advanced Light Source (ALS, Berkeley) and at PETRA III (DESY, Hamburg), initially the SAXS/WAXS/GISAXS/GIWAXS beamline 7.3.3 at the ALS, and beamline P03, the micro- and nano-focus small- and wide-angle X-ray scattering beamline (MiNaXS) at DESY.
The key components of our infrastructure comprise: pyFAI for azimuthal integration, gpCAM for optimization and uncertainty quantification, Tiled for unified data access, Prefect for workflow orchestration, and a Dash Plotly-based web-interface for initial configuration and monitoring during the experiment. We support reduction workflows for both transmission and grazing-incidence geometry and utilize machine-learning methods to extract the features that facilitate an autonomous loop.

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